Fthalide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 288 °C

Global applicability domain: Inside

Local applicability domain index: 3.72e-01

Confidence level: 5.16e-01

Nearest Neighbors from the Training Set

Image not found
Phosphine, ethyldiphenyl-
Measured: 293
Predicted: 310

Image not found
4-Bromobenzophenone
Measured: 350
Predicted: 336

Image not found
Diphenylsulfone
Measured: 279
Predicted: 315

Image not found
Phenyl phosphorodichloridate
Measured: 242
Predicted: 255

Image not found
1,3-Benzenedicarbonyl
dichloride
Measured: 276
Predicted: 279